LABORATORY FOR CHEMICAL TECHNOLOGY
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Supervisor(s)	**Period**	**Funding**
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Expansion, refinement and rationalization of industrial VGO hydrotreatment reactor simulation

Aim

Improving the simulation capabilities of the Single-Event MicroKinetics (SEMK) based trickle bed reactor model as available at the Laboratory for Chemical Technology (LCT) for more realistic, more complex feed by inclusion of hydrodenitrogenation (HDN) and hydrodesulphurization (HDS) reactions and deactivation kinetics.

Justification

A kinetic model for hydrocracking of Vacuum Gas Oils (VGOs) is available within a reactor model representative for industrial-scale operation. At present, the latter reactor model accounts for three-phase adiabatic operation in trickle flow. The underlying kinetics are described with a Relumped Single-Event MicroKinetic (RSEMK) model, considering, per carbon number, normal, mono-, di- and tri-branched paraffinic and mono-, di-, tri- and tetranaphthenic lumps. In addition, hydrogenation of mono-, di-, tri- and tetra-aromatic components is also accounted for. Catalyst deactivation was included in a pragmatic manner by the introduction of an incremental protonation enthalpy.
Although the model was capable of reproducing satisfactory the experimental data obtained on a pilot plant, some of the model features could be added or approached in a more fundamental manner in order to increase its predictive capabilities and interpretability, even for other, **more exotic VGO feeds**. The **addition of HDS and HDN kinetics was identified as vital** to increase the feed independence with respect to **N- and S- catalyst poisoning** and **deactivation**. Revisiting the thermodynamic and hydrodynamic methods was considered to be desirable to improve overall model predictive capabilities. An elaboration on more detailed hydrogenation and sequential cracking kinetics was also proposed but was expected to have a less significant impact on the model's predictive capabilities compared to the other actions listed in this paragraph.

Program

A one year program is scheduled in which an experienced post-doctoral research fellow will perform the following activities in order to reach the proposed project goals.

A. At present, the removal of nitrogen and sulphur components from the VGO feed is not simulated by the model, preventing the prediction of nitrogen and sulphur removal during hydrotreatment, critical to the properties of the fuel produced. Their occurrence (reversibly) impacts on the catalyst activity. A more correct assessment of their effect on the overall VGO hydrotreating kinetics will be achieved by **expanding the RSEMK model with HDN and HDS reactions**. The mechanism and corresponding kinetics for the HDN and HDS reactions to be implemented in the model will be decided upon after a **literature survey** and **cost/gain analysis**, i.e., implementation time and expected gain in model performance.
B. The different **catalyst deactivation and poisoning mechanisms under VGO hydrotreating conditions** will be reviewed. This review will allow to assess the **viability** of implementing these deactivation kinetics into the RSEMK model.
C. Lastly, the **updated RSEMK model will be tested** on its performance using other, **more exotic feedstocks**.